Title:

Interfacial thermodynamics of cryogenic fluids: The effect of non-condensable gas on fluid storage

Abstract:

Propellant tanks that contain cryogenic fluids (CFs) in low gravity conditions are usually pressurized with non-condensable (NC) gases for fast extraction. Unfortunately, the presence of NC gases causes CFs to exhibit higher boil-offs compared to pure CF systems. For optimal utilization of the cryogenic fuels, these higher boil-off rates must be minimized. Our goal is to quantify the effects NC gases have on the evaporation and condensation dynamics of CFs to develop strategies that mitigate the higher boil-offs. The hypothesis is that the NC gas accumulates around the CF's liquid vapor interface in the Knudsen layer, creating a kinetic barrier for both evaporation and condensation. Testing this hypothesis with experimental methods is difficult due to the transient nature of the Knudsen layer, which is only a few nanometers thick. Furthermore, experimental capabilities are limited in low gravity conditions and extremely expensive. Accordingly, we approach this problem from a theoretical perspective. In this study, we employ molecular dynamics (MD) simulations to probe the interfacial mechanisms that affect CF's evaporation and condensation at varying concentrations of NC gases. Specifically, we use nitrogen (N_2) and oxygen (O_2) as our CFs and neon (Ne) as our NC gas. Using MD simulations, we show that Ne accumulates at N_2 liquid vapor interface across a wide range of Ne concentrations, thereby impeding mass transport of N_2. Our simulations allow for direct computation of the molar flux as well as the mass accommodation coefficient (MAC) which can then be used as input parameters to continuum fluid dynamics (CFD) models for optimal storage tank design.